Strong-coupling Expansions at Finite Temperatures: Application to Quantum Disordered and Quantum Critical Phases

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Abstract

By combining conventional finite-temperature many-body perturbation theory with cluster expansions, we develop a systematic method to carry out high order arbitrary temperature perturbative calculations on the computer. The method is well suited to studying the thermodynamic properties of quantum disordered and quantum critical phases at finite temperatures. As an application, we calculate the magnetic susceptibility, internal energy and specific heat of the bilayer Heisenberg model. It is shown that for a wide range of coupling constants these expansions show excellent convergence at all temperatures. Comparing the direct series (without extrapolations) for the bulk susceptibility to Quantum Monte Carlo simulations we find an almost perfect agreement between the two methods even at the quantum critical coupling separating the dimerized and antiferromagnetic phases. The convergence fails only at very low temperatures, which are also difficult to reach by Quantum Monte Carlo simulations.

I. INTRODUCTION

Quantum critical phenomena and quantum disorder in strongly correlated many-body systems have been a subject of much interest lately. They have been invoked to account for many properties of high temperature superconductors[1], for non fermi-liquid behavior in heavy fermion materials[2], and for a variety of other interesting systems ranging from superconductor-insulator transitions to the quantum hall effect[3]. In many problems it is not possible to fine tune the system parameters to be right at the quantum critical point. Nevertheless, the quantum critical point controls their behavior above some very low temperature scale[4–6]. The aim of our study is to develop a method that will allow us to calculate the temperature dependence of thermodynamic quantities with high accuracy for many model Hamiltonians, when the system parameters are in the quantum disordered phase or near a zero temperature quantum critical point.

Quantum spin-systems provide a particularly rich variety of models and real materials where quantum critical phenomena can be studied. There exist many experimental realizations of spin-ladders and alternating chains[7]. Bilayer Heisenberg model is considered relevant to high temperature superconductors[8]. Recently, the material CaV_4O_9 has attracted considerable interest[9]. The spins in these materials are arranged in a novel geometrical arrangement, which allows for many possible types of spin-disordered ground states and quantum critical points.

Finite temperature properties of such systems have been studied before by finite-size studies, including exact diagonalization[10] and Quantum Monte Carlo simulations[11,12], and by high temperature expansions[13]. The latter method performs poorly at low temperatures for many parameter regimes of interest. Exact diagonalization, in higher than one dimension, is generally limited to fairly small systems and extrapolation to thermodynamic limit is unreliable. The Quantum Monte Carlo method is perhaps the most accurate to date, but it suffers from the sign problem when frustration is present.

Here, we combine many-body perturbation theory with cluster expansions to develop

high-order strong-coupling expansions for thermodynamic quantities, such as the bulk susceptibility and the specific heat, at arbitrary temperatures. The resulting series are perturbation expansions in the weaker couplings, whose coefficients depend on temperature. For the bilayer Heisenberg model, these series show excellent convergence at all temperatures for a range of parameters (without using series extrapolation methods such as Pade approximants). Even when the system parameters are tuned to the quantum critical point, the series converges very well down to fairly low temperatures, comparable to the lowest temperatures accessible in the Monte Carlo simulations.

The method should prove useful for frustrated as well as quenched random spin syatems. It can also be applied to electronic models such as t-J and Hubbard or Kondo lattice models. Being a finite temperature perturbation expansion, it is not limited to systems with non-degenerate ground states.

The plan of the paper is as follows: In section II we discuss the basic perturbation theory. In section III we introduce some techniques that are needed for an effective computer implementation of the method. In section IV the series expansions for the bilayer Heisenberg model is presented. In section V we compare our series with Quantum Monte Carlo simulations. Finally, in section VI we present our conclusions and suggest future directions.

II. PERTURBATION THEORY

We are interested in systems which are described by a Hamiltonian

$$\mathcal{H} = H_0 + \lambda H_1 \quad . \tag{1}$$

Here, H_0 consists of all couplings within an elementary cluster, whereas, H_1 describes interactions between different such units. The basic idea of cluster expansions is to exploit the fact that in any finite order of perturbation theory only a finite number of these elementary units can be coupled together and thus expansions for a thermodynamic system can be obtained exactly by carrying out perturbation theory just for these few finite-clusters

or graphs (In this paper we will refer to them as graphs to distinguish them from the elementary clusters which define the Hamiltonian H_0). A thermodynamic quantity, such as magnetic susceptibility per elementary cluster, χ, for the lattice $\mathcal{L}$ can be written as

$$\chi(\mathcal{L}) = \chi_0 + \sum_g L(g) \times W(g) \ . \tag{2}$$

Here χ_0 is the susceptibility of the elmentary cluster for $\lambda = 0$ and the sum runs over all connected graphs of the lattice. The quantity $L(g)$, called the lattice constant of the graph, is defined as the number of ways per elementary cluster that the graph g can be embedded in the lattice. The quantity $W(g)$ is the weight of the graph g defined by the recursion relation,

$$W(g) = \chi(g) - N_g\chi_0 - \sum_{g'} W(g') \ , \tag{3}$$

where, N_g is the number of sites in the graph and the sum over g' runs over all proper subgraphs of the graph g. For a graph g with B_g bonds it can be shown[14] that $W(g) = O(\lambda^{B_g})$.

So far the formalism is identical to a standard high temperature expansion. The novelty arises in the calculation of $\chi(g)$ for a finite graph. In order to do that, we only need to consider the spins in that graph and the interactions H_0 and H_1 between these spins. To calculate expansions at arbitrary temperature, we exploit the following relation

$$e^{-\beta(H_0+\lambda H_1)} = e^{-\beta H_0} \sum_n (-\lambda)^n I_n \ , \tag{4}$$

where I_n are n-fold integrals given by,

$$I_n = \int_0^\beta dt_1 \int_0^{t_1} dt_2 \ldots H_1(t_1)H_1(t_2)\ldots \tag{5}$$

Here, the operators, $H_1(t)$ have the standard time dependence of the interaction representation

$$H_1(t) = e^{tH_0} H_1 e^{-tH_0} \ . \tag{6}$$

Thus, the partition function can be reduced to the expression,

$$Z = Z_0 + \sum_{n=1} (-\lambda)^n Z_n \ \ , \tag{7}$$

where Z_n are given by

$$Z_n = \int_0^\beta dt_1 \int_0^{t_1} dt_2 \ldots Tr[e^{-\beta H_0} H_1(t_1) H_1(t_2) \ldots] \ \ . \tag{8}$$

It is evident that in order to evaluate these expressions, we need to work in a basis in which H_0 is diagonal. This basis is simply a direct product of the eigen-basis for elementary clusters. Thus calculating thermodynamic quantities is straightforward if the matrix elements of H_0 and H_1 are known in this basis. In the next section we discuss an efficient method for calculating these traces and integrals.

III. EVALUATING THE MULTIPLE INTEGRALS

The basic energy scale in this problem is set by the level spacing Δ_0 in the spectrum of the unperturbed part H_0. Measuring temperature in units of this quantity one finds that calculating Z_n requires repeated integrations over functions of type:

$$I(k, l; x_\nu) = x_\nu^k \ e^{l x_\nu} \tag{9}$$

Where k and l are integers and $k \geq 0$. It is then easy to see that the $I(k, l; x)$ form a closed set, because

$l \neq 0$:

$$\int_0^{x_{\nu-1}} dx_\nu \ x_\nu^k \ e^{l x_\nu} = k! \ \left(\frac{-1}{l}\right)^{k+1} + \sum_{i=0}^{k} (-1)^i \ \frac{1}{l^{i+1}} \ \frac{k!}{(k-i)!} \ x_{\nu-1}^{k-i} \ e^{l x_{\nu-1}} \tag{10}$$

$l = 0$:

$$\int_0^{x_{\nu-1}} dx_\nu \ x_\nu^k = \frac{1}{k+1} \ x_{\nu-1}^{k+1} \tag{11}$$

These equations allow for an iterative evaluation of the multiple integrals entering Eqn.(8). One finds that the coefficients Z_n are finite polynomials in the two variables $x = \Delta_0 / k_{\rm B} T$ and $y = \exp(-\Delta_0 / k_{\rm B} T)$.

In the following we will apply this series expansion method to systems where the basic cluster consists of a pair of $s = 1/2$ spins coupled by a Heisenberg exchange $J_\perp$. Thus, Δ_0 is the singlet-triplet spacing in the spectrum of H_0. In this case it turns out to be more convenient to use the variables (x, Z_0) instead of the variables (x, y), where $Z_0 = 1 + 3y$, is the zeroth order partition function.

IV. MODEL AND TABLES

Here, we apply the method to the spin-half bilayer Heisenberg model, defined by the Hamiltonian

$$\mathcal{H} = J_\perp \sum_i \mathbf{S}_{A,i} \cdot \mathbf{S}_{B,i} + J_\parallel \sum_{\langle i,j \rangle} \mathbf{S}_{A,i} \cdot \mathbf{S}_{A,j} + \mathbf{S}_{B,i} \cdot \mathbf{S}_{B,j} \tag{12}$$

Here, the index i enumerates sites on a two dimensional square lattice and $\langle i, j \rangle$ are pairs of nearest neighbour sites on this lattice. The expansion parameter is given by ratio of the inter dimer to the intra dimer coupling:

$$\lambda = J_\parallel / J_\perp \quad . \tag{13}$$

The series for the susceptibility χ and the logarithm of the partition function $\ln Z$ per dimer are presented in Tables 1 and 2. The series can also be obtained on the WWW. The acess adress is given at the end of this article.

V. RESULTS AND COMPARISONS

In this section we show the convergence of the expansions by comparing partial sums of different order and by comparing with the Quantum Monte Carlo data. It is known from a number of studies at $T = 0$ that this model has a quantum critical point at $\lambda \approx 0.4$[11,15]. We show here results in the quantum disordered phase (at $\lambda = 0.3$) and near the quantum critical point at $\lambda = 0.4$.

In figures (1) and (2) the susceptibility and specific heat are plotted as a function of temperature for $\lambda = 0.3$. One can see that there is excellent convergence at all temperatures.

The quantum critical regime was investigated by Chubukov, Sachdev and Ye[5] by a large-N expansion of the quantum nonlinear σ-model. They obtained very detailed results for the low temperature behaviour. In particular the following predictions for the susceptibility and the specific heat *per unit cell* were derived:

$$\chi = \frac{k_{\rm B}T}{(\hbar c)^2}\frac{\sqrt{5}}{\pi}\ln\left(\frac{\sqrt{5}+1}{2}\right)\left[1 - \frac{0.6189}{N} + O(N^{-2})\right] \tag{14}$$

$$C = \frac{3\zeta(3)}{\pi}k_{\rm B}\left(\frac{k_{\rm B}T}{\hbar c}\right)^2 N\left[\frac{4}{5} - \frac{0.3344}{N} + O(N^{-2})\right] \tag{15}$$

Where c is the spin wave velocity. From various zero temperature calculations its value is known to be[15]:

$$C = 1.90\ J_{\|} \tag{16}$$

Evaluating these equations for $N = 3$ gives for the susceptibility and specific heat *per site*:

$$\chi = \frac{1}{2\lambda^2}\ 0.272\ k_{\rm B}T \tag{17}$$

$$C = \frac{1}{2\lambda^2}\ 2.371\ k_{\rm B}\ (k_{\rm B}T)^2 \tag{18}$$

Here temperature is in units of the intra dimer coupling $J_{\perp}$.

A very sensitive measure for quantum criticality is the Wilson ratio defined by

$$W = \frac{k_{\rm B}^2 T\ \chi(T)}{C(T)}. \tag{19}$$

The numerical value of this dimensionless quantity follows immediately from Eqns.(17) and (18):

$$W = 0.115 \quad . \tag{20}$$

In figures 3, 4, 5, and 6, the susceptibility, internal energy, specific heat, and Wilson ratio for the model are shown and compared with Monte Carlo data and with the asymptotic quantum critical predictions. We see that the series converges extremely well down to fairly

low temperatures. However, the convergence appears to break down just as the asymptotic quantum critical behavior sets in. The finite series become oscillatory at these very low temperatures. The activated behaviour at extremly low temperatures as seen in figures 3, 5 and 6 is also an artifact of finite series. In principle various extrapolation techniques, e.g. Pade approximants, can be used to enhance the convergence in this region. Here, we restrict the analysis to the temperature range where the series converge.

One interesting result to emerge from this study is that asymptotic quantum critical scaling occurs in the model only at very low temperatures, much lower than anticipated before. The uniform susceptibility between $T = 0.1J_\perp$ and $T = 0.4J_\perp$ appears nearly linear but is not strictly so. There is a shoulder around $T = 0.2J_\perp$, which is present in both the series results and the Monte Carlo data.

On the other hand, many amplitude ratios follow the universal quantum critical predictions even above $T = 0.1J_\perp$[12]. Thus, the extent of the quantum critical regime in 2D systems appears to strongly depend on the quantity studied. Clearly, the role of lattice corrections needs to be better understood[16].

VI. CONCLUSIONS AND FUTURE DIRECTIONS

In this paper we presented a practical method to calculate high order strong coupling expansions for quantum statistical models at arbitrary temperatures. The method was applied to the bilayer Heisenberg model, where it shows excellent convergence even near the quantum critical point. In a companion paper, we will discuss application of these methods to alternating spin-chains and spin-ladders. The method is also applicable to frustrated and quenched random spin models as well as to Hubbard or Kondo models around the strong coupling limit. We are preparing to pursue these calculations in the future.

Series for the susceptibility χ, internal energy E and specific heat C may be obtained on the WWW. In addition a Fortran program to read the data files and sum the series is also available.

The WWW access is via http://brahms.physik.uni-bonn.de/~ norbert/series/series.html

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FIGURES

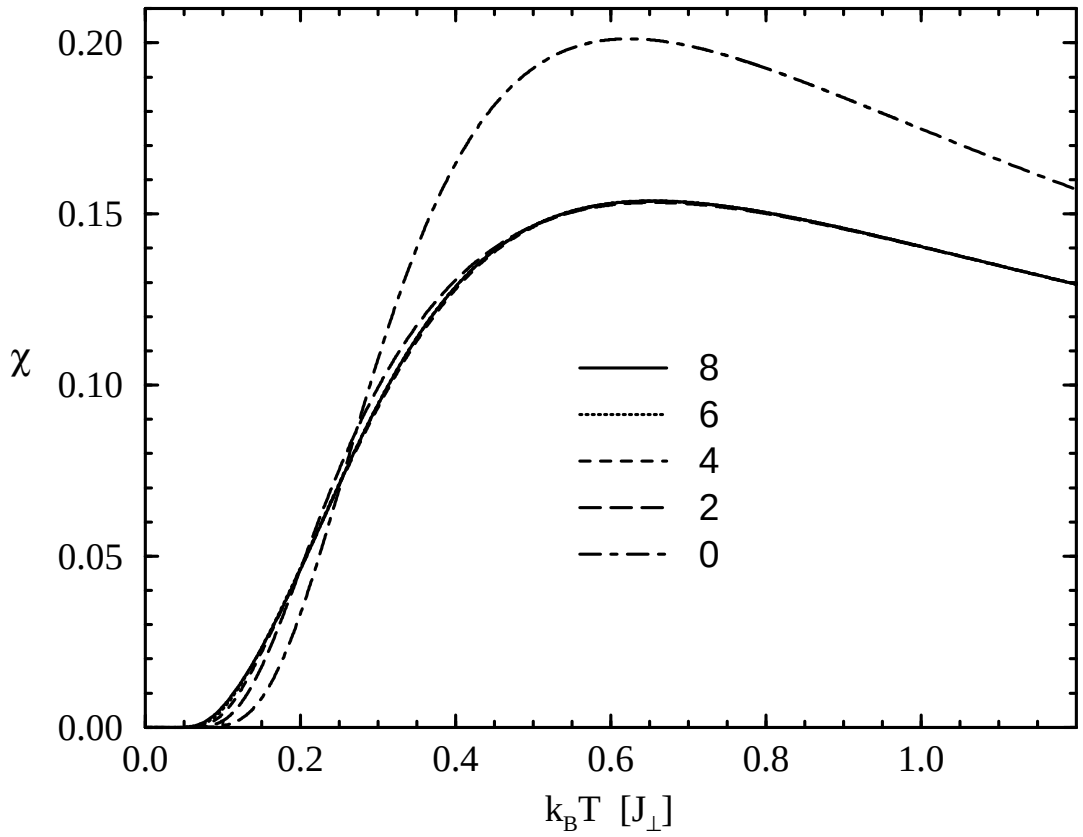

FIG. 1. Susceptibility χ per spin vs. temperature $k_{\rm B}T/J_\perp$ for $J_\parallel/J_\perp = 0.3$, i.e. in the quantum disordered regime. The lines are series of order 2, 4, 6 and 8 compared to the susceptibility of an isolated dimer (0).

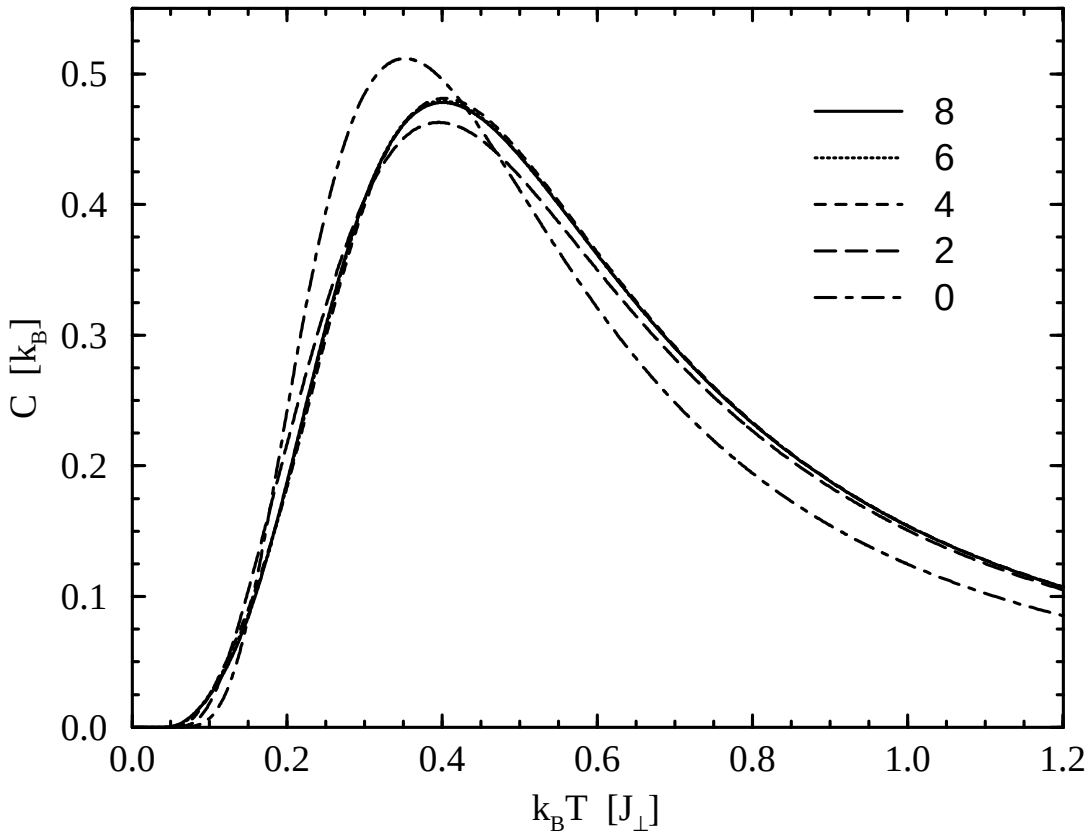

FIG. 2. Specific heat C per spin vs. temperature $k_{\rm B}T/J_\perp$ for $J_\parallel/J_\perp = 0.3$, i.e. in the quantum disordered regime. The lines are series of order 2, 4, 6 and 8 compared to the specific heat of an isolated dimer (0).

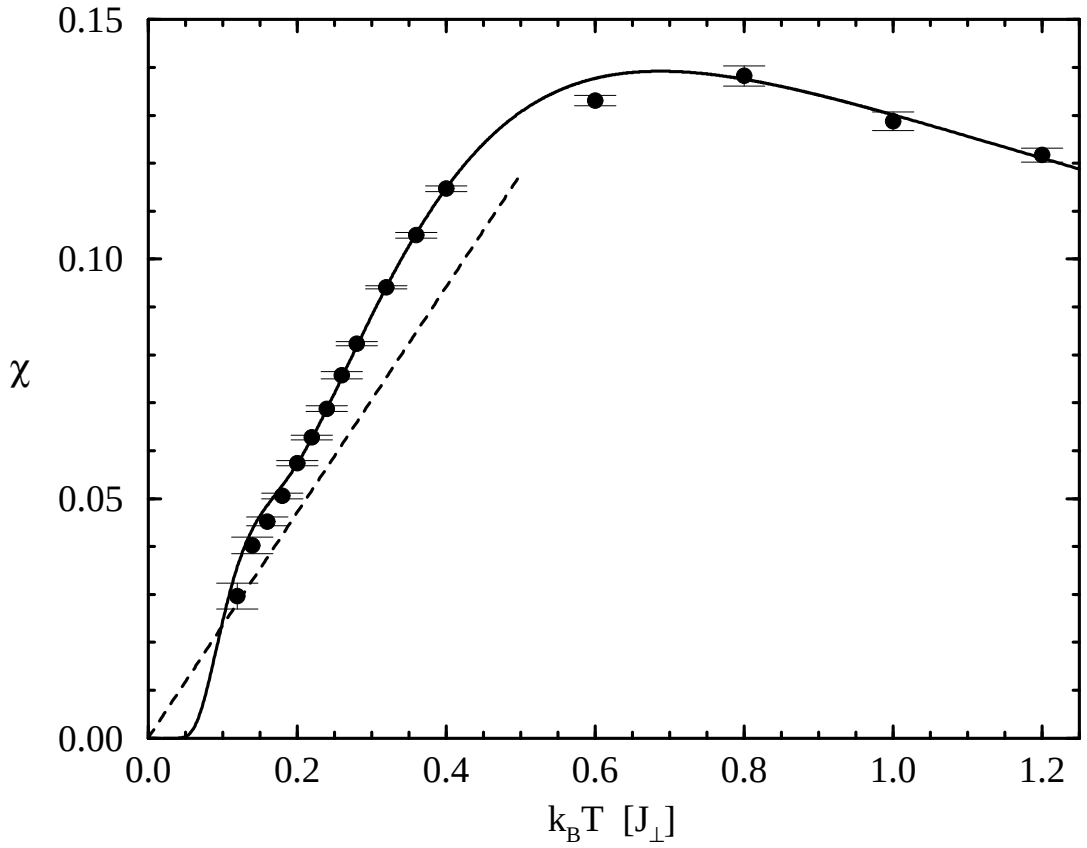

FIG. 3. Susceptibility χ per spin vs. temperature $k_{\rm B}T/J_\perp$ for $J_\parallel/J_\perp = 0.4$, i.e. close to the quantum critical point. The black circles show the QMC data of Sandvik and Scalapino. The solid lines is the series of order 8. The dashed line is the quantum critical (QC) prediction of Eqn. (17)

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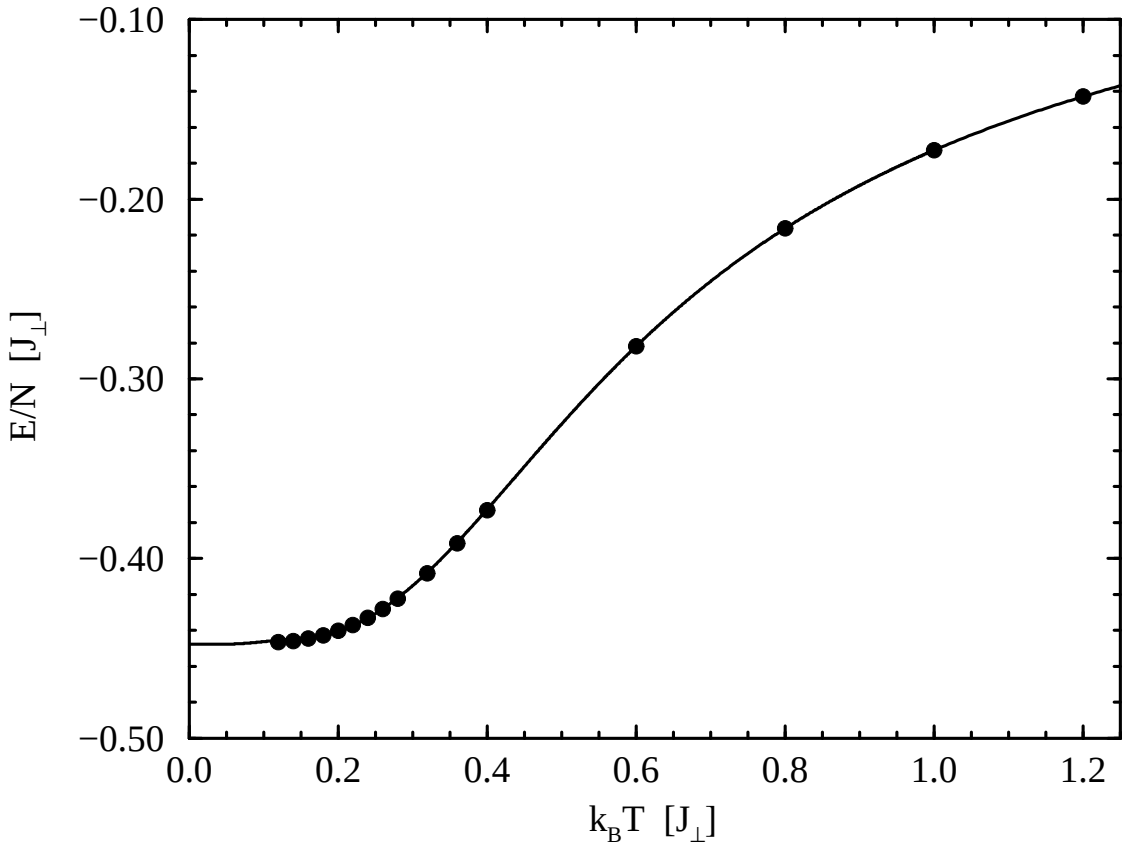

FIG. 4. Internal Energy per spin $E/NJ_\perp$ vs. temperature $k_{\rm B}T/J_\perp$ for $J_\parallel/J_\perp = 0.4$. The line is the series up to order 8. The black dots show the QMC data of Sandvik and Scalapino.

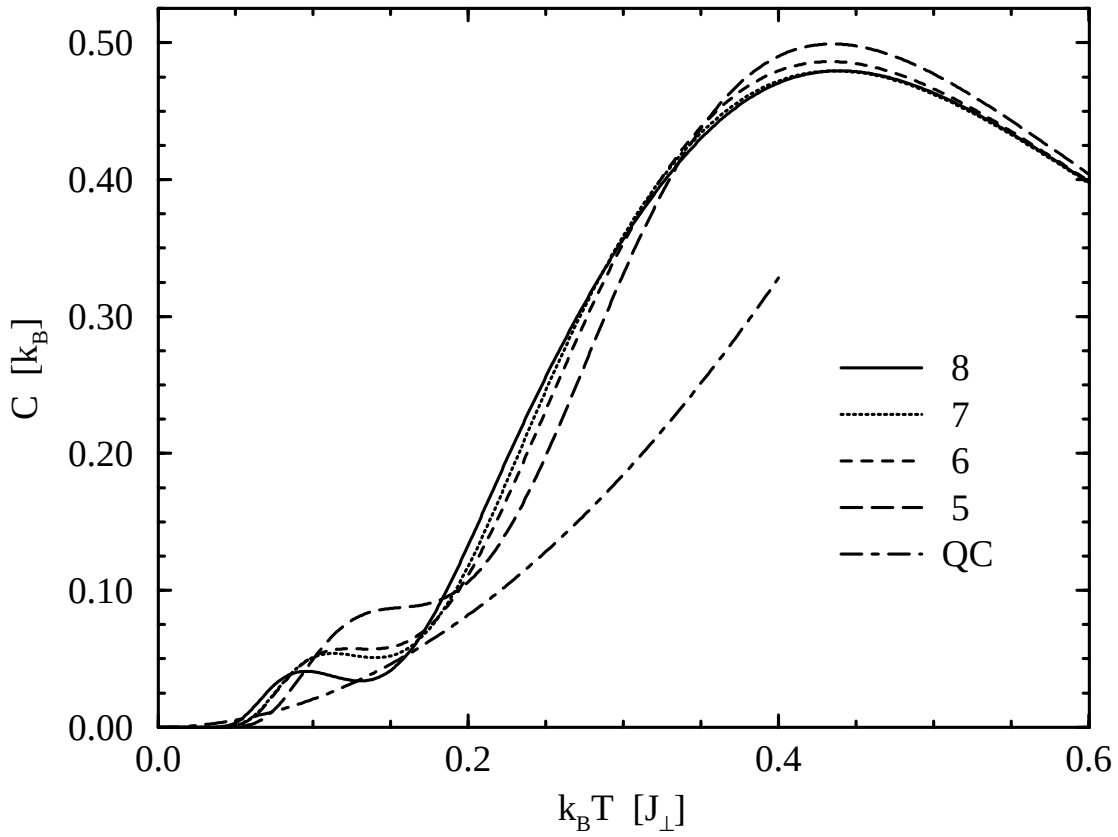

FIG. 5. Specific heat per spin C vs. temperature $k_{\rm B}T/J_\perp$ for $J_\parallel/J_\perp = 0.4$. The lines are series of order 5, 6, 7 and 8 and the quantum critical (QC) prediction of Eqn. (18) .

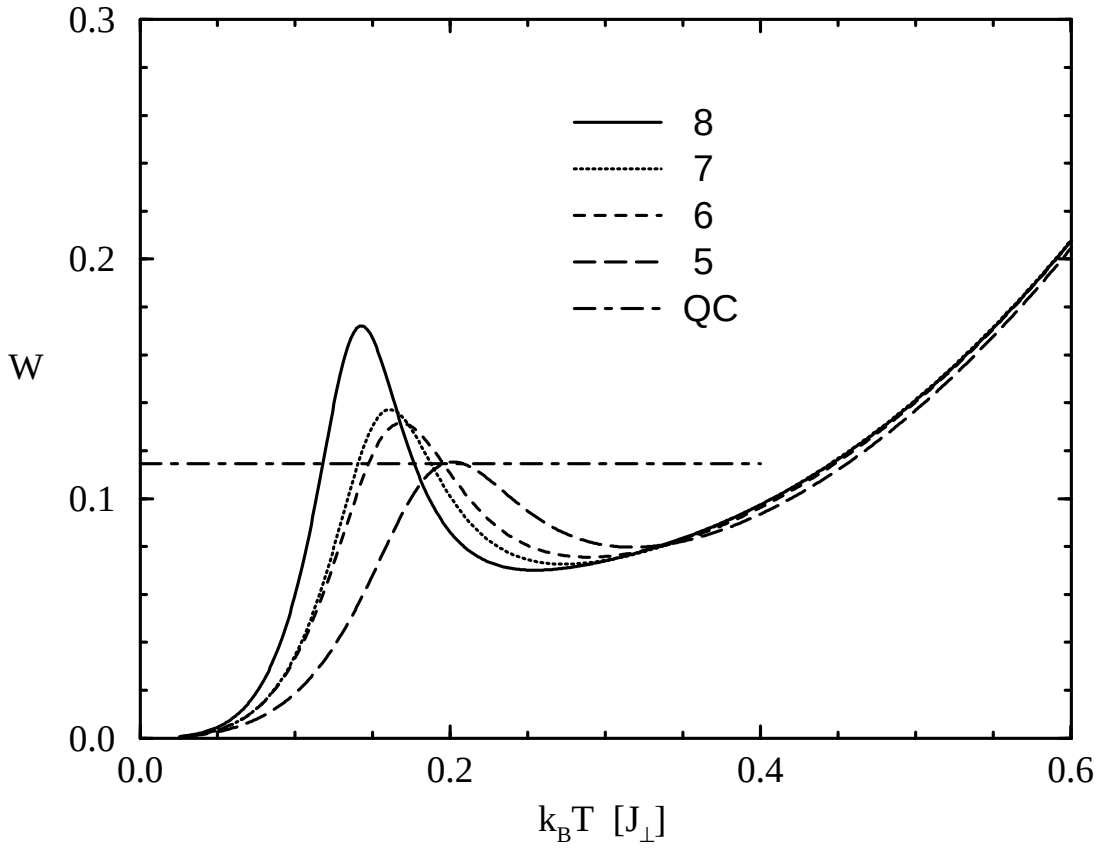

FIG. 6. Wilson ratio W vs. temperature $k_{\rm B}T/J_\perp$ for $J_\parallel/J_\perp = 0.4$. W obtained from series for χ and C of order 5, 6, 7 and 8 and compared to the quantum critical (QC) prediction of Eqn. (20)

.

Table 1.: Series for the bulk susceptibility χ per dimer

$$\chi_u(\lambda;\beta) = \frac{1}{12}\sum_{n=0}(-\lambda)^n \frac{1}{12^n n!}\chi_n(\beta) \qquad \text{with} \qquad \chi_n(\beta) = \sum_{k=0}^{n}\sum_{l=0}^{n+1} c_{kl}\beta^k Z_0^{-l}.$$

Here $Z_0 = 1 + 3\exp(-\beta)$ is the partition function of an isolated dimer.

χ_0:

	1
0	8
1	-8

χ_1:

l\k	2
0	128
1	-256
2	128

χ_2:

l\k	2	3
0	384	2688
1	-1152	-8064
2	-2304	9216
3	3072	-3840

χ_3:

l\k	2	3	4
0	-6912	18432	73728
1	20736	-87552	-308736
2	41472	-138240	571392
3	-55296	465408	-511488
4	0	-258048	175104

χ_4:

l\k	2	3	4	5
0	787968	428544	912384	2370048
1	-4280832	-2032128	-4396032	-11976192
2	2497536	14515200	-6027264	28821504
3	13381632	-42771456	41969664	-40270848
4	-24182784	51093504	-54577152	30504960
5	11796480	-21233664	22118400	-9449472

χ_5:

l\k	2	3	4	5	6
0	-57646080	14837760	29767680	44605440	87932928
1	346982400	-165703680	-195010560	-221921280	-476614656
2	-273576960	-428359680	1591050240	-441077760	1352337408
3	-1213470720	3835146240	-6198865920	3826851840	-2642288640
4	1976279040	-7331604480	11384985600	-7836364800	3361351680
5	-778567680	5491261440	-9726197760	6798458880	-2349711360
6	0	-1415577600	3114270720	-2170552320	666992640

χ_6:

l\k	2	3	4	5	6	7
0	12918528000	7489013760	4882083840	2302248960	2285660160	3858315264
1	-83086663680	-37391155200	-29798461440	-16123207680	-13725573120	-23258603520
2	112199178240	219853854720	-64553656320	138725775360	-22857431040	71384205312
3	145302958080	-829322219520	682678886400	-639576207360	278069760000	-155211411456
4	-506555596800	1734012334080	-1915608268800	1637361561600	-784237731840	258483916800
5	696756142080	-2181593088000	2706940477440	-2308508467200	1093588992000	-294514016256
6	-591569879040	1553242521600	-1938315018240	1653277409280	-767088230400	190193614848
7	214035333120	-466291261440	553773957120	-467459112960	213964554240	-50936020992

χ_7:

l\k	2	3	4	5	6	7	8
0	-2213251568640	-495870197760	327807406080	350493696000	169998151680	133894397952	188246827008
1	14563573355520	1073517096960	-2334586060800	-2449236787200	-1446944808960	-920540823552	-1267894665216
2	-21593862420480	-27276743208960	34889907548160	-7746371297280	11662847078400	-207016943616	3808230875136
3	-23096475924480	140663776296960	-173864730009600	95048378449920	-63978511564800	16089805799424	-7204267671552
4	100188984913920	-337715756421120	467620165877760	-348518405652480	214780183511040	-65438937317376	12744739897344
5	-132076661391360	476530149150720	-768271630049280	683237322915840	-426119730462720	136632715591680	-22588348317696
6	90411348787200	-401291848581120	752002630041600	-755460220354560	483148426199040	-160560949248000	27719857815552
7	-26183655751680	182473048719360	-395769662668800	440930622504960	-288393102950400	99145204236288	-18112389120000
8	0	-33960272855040	85400097914880	-105392583475200	70176834846720	-24874175692800	4711824359424

χ_8:

l\k	2	3	4	5	6	7	8	9
0	767385761587200	464776262737920	168561479761920	60667304140800	24452127866880	9493653012480	8024287444992	9676674736128
1	-5144624913899520	-2502379210383360	-1060697318768640	-439772371476480	-159448473354240	-67066129170432	-55243334909952	-70524198641664
2	8362808833720320	1408491735625920	-384656446699520	4863113478881280	-712029843947520	589633843986432	27836124954624	240374538141696
3	5408213862481920	-50809847032627200	36584709979668480	-28534912647413760	10370107357102080	-4344471627890688	902233114804224	-492429718241280
4	-31791683395584000	111435849584640000	-117116006702284800	96719011517399040	-47526121829007360	19323886990786560	-4677680996352000	751044776067072
5	46254298890240000	-169364987105771520	226318548946452480	-210111477981511680	121845160399011840	-51956976934453248	12837450214342656	-1303538324668416
6	-48823359048253440	196736261750784000	-294878887018168320	299746770571100160	-191673002645913600	85653737241182208	-21795082473701376	2385672663859200
7	49936417098301440	-172757768931901440	256218116149739520	-270626527382077440	182583729759191040	-84307372280119296	22333003678089216	-2889346648375296
8	-37157865605038080	97634880753500160	-133154075993702400	138989349025873920	-96085732648550400	45255520844513280	-12481243632893952	1829730623422464
9	12188408516444160	-24921703427604480	30766294924001280	-30666221514915840	21332885797601280	-10156385601847296	2900703018221568	-460660386299904

Table 2.: Series for the logarithm of the partition function $\ln Z$ per dimer

$$\ln Z(\lambda;\beta) = \ln Z_0 + \sum_{n=1} (-\lambda)^n \frac{1}{12^n n!} f_n(\beta) \qquad \text{with} \qquad f_n(\beta) = \sum_{k=0}^{n} \sum_{l=0}^{n+1} c_{kl} \beta^k Z_0^{-l}.$$

Here $Z_0 = 1 + 3\exp(-\beta)$ is the partition function of an isolated dimer.

f_2:

l\k	1	2
0	-24	96
1	48	-48
2	192	-48

f_3:

l\k	1	2	3
0	432	864	-288
1	-864	-1728	576
2	-3456	864	-288

f_4:

l\k	1	2	3	4
0	-41760	-55296	-13824	-2304
1	158400	160704	-24192	-77760
2	138240	-430272	10368	205632
3	-506880	988416	-110592	-122112
4	368640	-663552	138240	-3456

f_5:

l\k	1	2	3	4	5
0	2859840	4199040	2782080	103680	109440
1	-12476160	-17210880	-10091520	1105920	668160
2	-6324480	38413440	10938240	2799360	-2609280
3	47969280	-56920320	-864000	-9331200	2776320
4	-24330240	31518720	-2764800	5322240	-944640

f_6:

l\k	1	2	3	4	5	6
0	-569462400	-672675840	-310832640	-63452160	6220800	-6220800
1	2689459200	2966492160	1260126720	296524800	70917120	183831552
2	-156245760	-8726745600	-187453440	7464960	-673505280	-444552192
3	-7881960960	16105236480	-5395921920	-610053120	2198845440	-16312320
4	9728501760	-23978488320	15582689280	-1792005120	-2801848320	741325824
5	-9289728000	24020582400	-19654410240	4663111680	1186099200	-518676480
6	4459069440	-9714401280	8705802240	-2501591040	13271040	60604416

f_7:

l\k	1	2	3	4	5	6	7
0	89047395360	110724485760	58990498560	16056714240	-672053760	-721405440	116024832
1	-440447414400	-531234547200	-287505469440	-81453496320	3779758080	675827712	-6399074304
2	117483307200	1579679781120	317464842240	85326151680	814302720	-17347696128	21352536576
3	1279789580160	-2813668462080	422485217280	-152130908160	20591262720	31405667328	-21181160448
4	-1955637250560	3737580900480	-1687259185920	495232496640	-146069360640	28659972096	-1691698176
5	1533362503680	-3133193011200	1945478062080	-555514122240	209889792000	-81196867584	12815953920
6	-545492828160	1050110853120	-769653964800	192483164160	-88333701120	38524502016	-5012582400

f_8:

l\k	1	2	3	4	5	6	7	8
0	-28664815818240	-32591048232960	-14499570032640	-3021936906240	-239733043200	177006477312	26531463168	12850679808
1	144608849925120	155543330073600	68811924142080	17838829532160	1926486374400	-2269960132608	-514036518912	-249380305920
2	-60794389555200	-518632755379200	-59806624389120	-30553999580160	-13546484582400	10249704105984	3478877982720	-918892071936
3	-366285335592960	1025042394378240	-223731649290240	83800325468160	46315773665280	-42114884345856	-7230439931904	8011031556096
4	639727016140800	-1416307344076800	828567910195200	-312900967249920	-75109982330880	126097177006080	-4625486659584	-15544549767168
5	-579394111242240	1661222905896960	-1523031536517120	748914182553600	7577120194560	-200735322439680	34784356368384	10164135444480
6	517910510960640	-1681713886003200	1851925113077760	-1122885281710080	166439411712000	149237092859904	-44402769395712	819762315264
7	-442482378670080	1196838019399680	-1343036042772480	912495052062720	-217829258035200	-36727534190592	21548808142848	-2844450422784
8	190443883069440	-389401616056320	414800475586560	-293686204170240	84466666045440	-3913279340544	-3065841451008	549492572160